

The ATHAS Data Bank of Heat Capacities of Polymers

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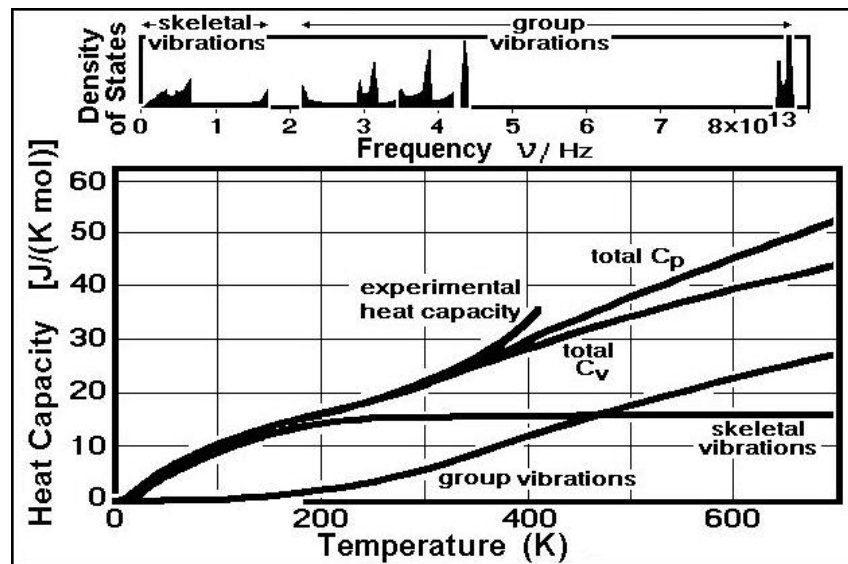
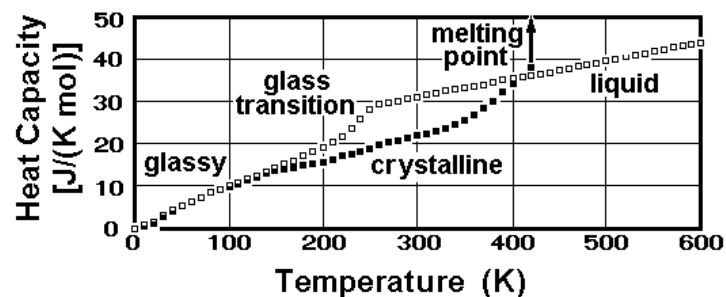
DMR 77-11377, 83-17097, 88-18412, 90-00520, and 97-03692

In the 20th century polymers have replaced metals as the most important material needed for society. A polymer molecule consists of thousands of atoms, bound to a flexible chain. Large numbers of these molecules can easily be shaped into objects with liquid, elastic, or solid properties. In 1980, work was begun on the **ATHAS Data Bank** (Advanced Thermal Analysis System). It contains information on thermal properties of over 200 polymers, and was collected or measured with help from the above listed grants over the last 25 years. It is the first and only such table for polymers.

The top Figure shows data for the well-known polyethylene (CH_2)_x. The heat capacity has, in addition, been linked to the molecular motion, as sketched in the bottom Figures. Note the enormously fast motion and some gradual deviations in heat capacity.

Heat Capacities of Amorphous (Glassy and Liquid) and Crystalline Polyethylene

Collected, averaged, and extrapolated from over 100 sets of literature data



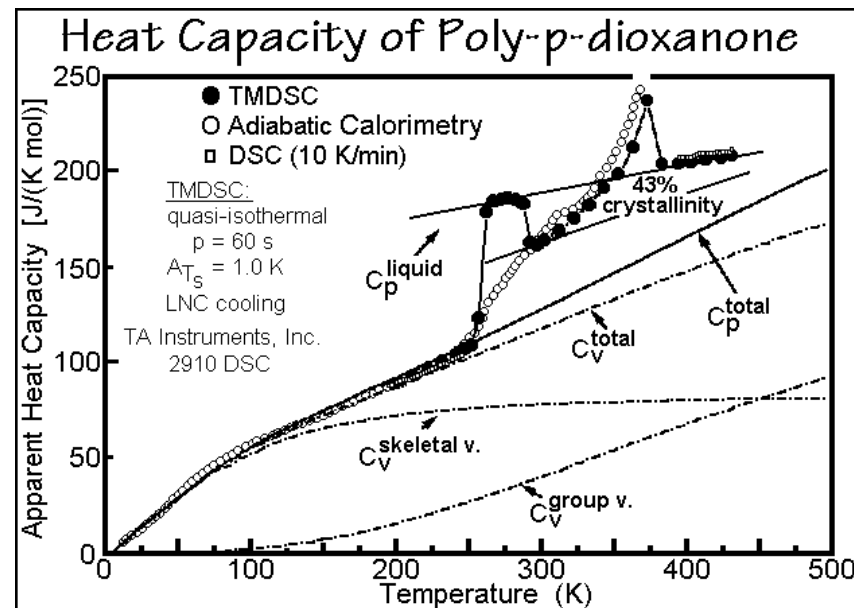
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The Intellectual Merit of this research lies in the growth of understanding of molecular structures and their motion. One needs to magnify the molecular structure by a factor of 10,000 in order to get to the human, macroscopic scale. The molecular motion is a billion times faster than the human time scale. While knowledge about structure was gained already in the 20th century, both must be understood for the 21st. The figure on the right shows an example of the the Data Bank allowing assignment of motion and thermal properties for a new polymer. A full model of the defect state of polymers has been derived based on such thermal properties.

The Broader Impact and Teaching of this long-range project is based on the availability of the data bank *via* the internet, and the concept of structure and motion is available without charge in form of the computer-based course entitled



Thermal Analysis of Polymeric Materials which consists of more than 2,500 computer screens. Both can be found in downloadable form on the **ATHAS** web-site which has been visited more than 25,000 times over the last five years (web.utk.edu/~athas). See also: BW *Prog. Polymer Sci.*, **28**, 384-450 (03). BW *et al.*, *Adv. Polymer Sci.*, **116**, 27-72 (94).